New Compounds

Some Semicarbazones and Thiosemicarbazones[1]

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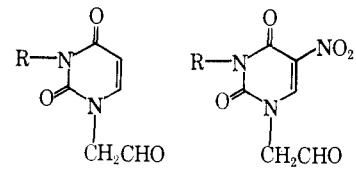
A number of semicarbazones and thiosemicarbazones of aromatic and heterocyclic aldehydes have been examined for antiviral and antitumor activities[2] since Brockman, *et al.*,[3] first observed the antileukemic effect of 2-formylpyridine thiosemicarbazone. In a search for other antitumor agents of this type, we have converted the aldehydes **1–5**, which were available from other studies, to the derivatives listed in Table I.

TABLE I
DERIVATIVES OF ALDEHYDES **1–5**

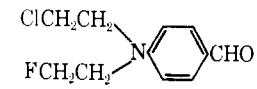
RCHO	Deriv.[a]	Yield, %	Mp, °C	Formula	Calcd, % C	Calcd, % H	Calcd, % Other	Found, % C	Found, % H	Found, % Other
1	M	95	243.5–244.0	$C_8H_{11}N_5O_2S$	39.8	4.60	*S*, 13.3	39.7	4.56	*S*, 13.4
	S	100	225.0–225.5	$C_7H_9N_5O_3 \cdot 0.5H_2O$	38.2	4.58		38.2	4.83	
	T	78	223–228[b]	$C_7H_9N_5O_2S$	37.0	3.98		37.0	4.21	
2	S	67	229–230	$C_{10}H_{14}N_8O_4$	38.7	4.54		39.0	4.66	
	T	72	225–227	$C_{10}H_{14}N_8O_2S_2$	35.1	4.12		34.9	4.19	
	M	60	215–216	$C_{12}H_{18}N_8O_2S_2$	38.9	4.99	*S*, 17.3	38.7	5.05	*S*, 17.1
3	S	100	250.0–250.5	$C_{11}H_8N_6O_5$	32.8	3.15	*N*, 32.8	32.9	3.30	*N*, 32.8
	M	82	206–210	$C_8H_{10}N_6O_2S$	33.6	3.52	*N*, 29.4	33.3	3.76	*N*, 29.3
	T	86	238–240	$C_{11}H_8N_6O_4S$	30.9	2.95		31.0	3.10	
4	M	67	225–227[b]	$C_{12}H_{12}N_8O_4S_2$	34.7	4.13	*N*, 30.2	34.5	3.91	*N*, 29.9
5	T	70	153–155	$C_{12}H_{16}ClFN_4S_2$	47.6	5.32	*N*, 18.5	47.8	5.74	*N*, 18.2
	M	59	135–136	$C_{13}H_{18}ClFN_4S$	49.2	5.73	*N*, 17.7	48.8	6.03	*N*, 18.0

[a] The types of derivatives are: M, N⁴-methylthiosemicarbazone; *S*, semicarbazone; T, thiosemicarbazone. For **2** and **4**, the dialdehydes, these stand for the bis derivatives. [b] Recrystallized from aqueous *N*,*N*-dimethylformamide.



1, R = H
2, R = CH_2CHO

3, R = H
4, R = CH_2CHO



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Experimental Section

The semicarbazone-type derivatives were prepared by the usual procedure.[4] The derivatives were all crystallized from or washed with ethanol or aqueous ethanol, except as noted.

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Trifluoromethylbenzaldoximes[1]

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Oximes exhibit skeletal muscle relaxant activity.[3] Preliminary pharmacological screening has shown that *m*-trifluoromethylbenzaldoxime has this action.[4] This series of compounds (see Table I) was synthesized so that the relationship of the oxime configuration and the trifluoromethyl substituent position to the pharmacological potency could be evaluated.

Experimental Section

Trifluoromethylbenzaldehydes.—The corresponding trifluoromethylbenzonitriles[5] were converted to the aldehydes by reaction

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(4) Decreased locomotor activity and muscle tone of the trunk and limbs was observed in mice at 32 mg/kg iv with an MED_{50} of 18 mg/kg iv. The pharmacological screening was conducted by the Toxicity Screening Branch, U. S. Army Edgewood Arsenal, Md., to whom the authors are indebted.